Investigations on the Use of NMR Spectroscopy for Structural Determinations in the Field of Polycyclic Aromatic Substances

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Up to now, very little use has been made of NMR spectroscopy in the field of polycondensed aromatics.

A systematic investigation of

1--unsubstituted polycyclic aromatic hydrocarbons,
2--polycondensed aza-aromatic systems,
3--monosubstituted derivatives of triphenylene, phenanthrene, biphenylene, benzo[a]biphenylene, pyrene, benzo[c]phenanthrene, dibenzo[g,p]chrysene (tetrabenzonapthalene), fluorene and acenaphthene,
4--aromatic cyclic ketones,

has yielded information which can be used to solve many structural problems resulting from ambiguous syntheses.

Screening effects (shielding and deshielding of aromatic protons) due to substituents and cyclic heteroatoms are particularly important in ortho, meta, para, peri and "angular" positions. The precise knowledge of these effects and of their magnitude is, of course, of great importance for the interpretation of integrated spectra of unknown substances.

The scope and limitations of this technique will be discussed and illustrated by examples drawn from the chemistry of polycyclic aromatic hydrocarbons and polycondensed heterocyclic compounds.